

Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Magnetic properties in the Mott-insulating iron oxychalcogenides

La₂O₂Fe₂OSe₂¹ JIAN-XIN ZHU, Theoretical Division, Los Alamos National Laboratory, Los Alamos, NM 87545, RONG YU, QIMIAO SI, Department of Physics & Astronomy, Rice University, Houston, TX 77005 — The role of electron correlation and magnetism in high-temperature superconductivity of the iron pnictides has been a topic of discussion. It has also motivated interest to compare related compounds with the iron pnictides and chalcogenides. Recently both electronic structure calculations and experimental measurements have indicated that the iron oxychalcogenides La₂O₂Fe₂OSe₂, which contains an Fe square lattice with an enlarged unit cell, has a larger U/t and is a Mott insulator [1]. We focus here on the understanding of the magnetism of this system. Within the density functional theory, we consider the magnetic phase diagram. Using an effective frustrating spin-exchange model in a doubled checker-board lattice, we study the magnetic excitation spectrum. Our theoretical results are compared with the emerging elastic and inelastic neutron scattering data in this compound.

[1] J.-X. Zhu, R. Yu *et. al.*, Phys. Rev. Lett. **104**, 216405 (2010).

¹This work was supported by the NNSA of the U.S. DOE at LANL under Contract No. DE-AC52-06NA25396 (J.X.Z), the NSF Grant No. DMR-0706625, the Robert A. Welch Foundation Grant No. C-1411, and the W. M. Keck Foundation (R.Y. and Q.S.).

Jian-Xin Zhu
Theoretical Division, Los Alamos National Laboratory,
Los Alamos, NM 87545

Date submitted: 30 Dec 2010

Electronic form version 1.4